

Typical Product Specifications & Properties

(±)-2-(4-chlorophenyl)benzoxazole-5-propionic acid

CAS Number: : 67434-14-4

Specifications	Limits
EINECS	266-692-3
SMILES	<chem>c12c(oc(n1)c1ccc(Cl)cc1)ccc(c2)[C@@H](C(O)=O)C</chem>
InChI	MITFXPHMIHQXPI-UHFFFAOYSA-N
InChIKey	1S/C16H12ClNO3/c1-9(16(19)20)11-4-7-14-13(8-11)18-15(21-14)10-2-5-12(17)6-3-10/h2-9H,1H3,(H,19,20)
Henry's Law Constant	4.26E-13 atm-m3/mole
log P (octanol-water)	3.23
Vapor Pressure	5.26E-09 mm Hg
Atmospheric OH Rate Constant	1.68E-11 cm3/molecule-sec
Water solubility	52 mg/L